

10/525,906

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NEWS	2	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	3	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	4	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	12	JUN 25	CA/CAPLUS and USPAT databases updated with IPC reclassification data
NEWS	13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	17	JUL 28	CA/CAPLUS patent coverage enhanced
NEWS	18	JUL 28	EPFULL enhanced with additional legal status information from the EPOLINE Register
NEWS	19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	20	JUL 28	STN Viewer performance improved
NEWS	21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	22	AUG 13	CA/CAPLUS enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	24	AUG 15	CAPLUS currency for Korean patents enhanced
NEWS	25	AUG 25	CA/CAPLUS, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS	26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	27	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	28	SEP 25	CA/CAPLUS current-awareness alert options enhanced to accommodate supplemental CAS indexing of

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exemplified prophetic substances
NEWS 29 SEP 26 WPIDS, WPINDEX, and WPIX coverage of Chinese and
and Korean patents enhanced
NEWS 30 SEP 29 IFICLS enhanced with new super search field
NEWS 31 SEP 29 EMBASE and EMBAL enhanced with new search and
display fields

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:12:58 ON 29 SEP 2008

=> file reg

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FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 26 SEP 2008 HIGHEST RN 1053621-88-7

DICTIONARY FILE UPDATES: 26 SEP 2008 HIGHEST RN 1053621-88-7

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

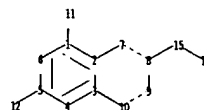
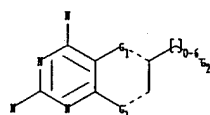
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=>

Uploading C:\Program Files\Stnexp\Queries\10525906a.str



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chain nodes :
11 12 15 16 17 18 19 20 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
1-11 5-12 8-15 15-16 17-18 17-19 20-21 21-22
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10
exact/norm bonds :
1-11 2-7 3-10 5-12 7-8 8-9 8-15 9-10 15-16 17-18 17-19 20-21 21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

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G1:C,N

G2:[*1],[*2]

Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS

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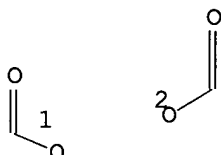
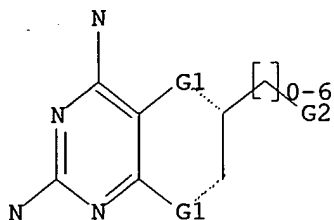
L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR

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G1 C,N

G2 [G1], [G2]

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:13:29 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 723 TO ITERATE

100.0% PROCESSED 723 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 12847 TO 16073

PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:13:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 13950 TO ITERATE

100.0% PROCESSED 13950 ITERATIONS

182 ANSWERS

SEARCH TIME: 00.00.01

L3 182 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

178.57

FILE 'CAPLUS' ENTERED AT 15:13:44 ON 29 SEP 2008

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FILE COVERS 1907 - 29 Sep 2008 VOL 149 ISS 14
FILE LAST UPDATED: 28 Sep 2008 (20080928/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s 13

L4 100 L3

=> s 14 and (benzoylamino or benzamide)

2865 BENZOYLAMINO

22119 BENZAMIDE

L5 0 L4 AND (BENZOYLAMINO OR BENZAMIDE)

=> s 14 and pentane?

73880 PENTANE?

L6 0 L4 AND PENTANE?

=> s 14 and (carboxyl? or petanedioic)

434115 CARBOXYL?

0 PETANEDIOIC

L7 16 L4 AND (CARBOXYL? OR PETANEDIOIC)

=> d 17 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 16 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:86232 CAPLUS

DOCUMENT NUMBER: 146:184481

TITLE: Preparation of pyrido[2,3-d]pyrimidine-2,4-diamine derivatives as PTP1B inhibitors

INVENTOR(S): Berthel, Steven Joseph; Cheung, Adrian Wai-Hing; Kim, Kyungjin; Li, Shiming; Thakkar, Kshitij Chhabilbhai; Yun, Weiya

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 132pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007009911	A1	20070125	WO 2006-EP64091	20060711
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GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

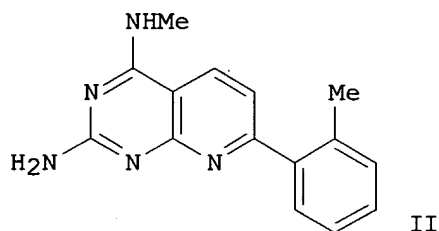
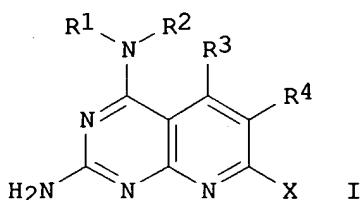
AU 2006271809 A1 20070125 AU 2006-271809 20060711
 CA 2614443 A1 20070125 CA 2006-2614443 20060711
 EP 1910359 A1 20080416 EP 2006-777692 20060711

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR

US 20070021445 A1 20070125 US 2006-488863 20060718
 KR 2008018957 A 20080228 KR 2008-701454 20080118
 MX 200800885 A 20080318 MX 2008-885 20080118
 IN 2008DN00656 A 20080711 IN 2008-DN656 20080124
 CN 101243081 A 20080813 CN 2006-80029809 20080215

PRIORITY APPLN. INFO.: US 2005-701467P P 20050721
 WO 2006-EP64091 W 20060711

OTHER SOURCE(S): MARPAT 146:184481
 GI



AB Title compds. represented by the formula I [wherein X = (un)substituted Ph, heteroaryl or cycloalkyl; R1, R2 = independently H, (methoxy)alkyl or hydroxyalkyl; R3 = H, alkyl or phenyl; R4 = H, alkyl(sulfonyl), Ph or carboxy; and pharmaceutically acceptable salts or esters thereof] were prepared as PTP1B inhibitors. For example, II was provided in a multi-step synthesis starting from the reaction of 2'-methylacetophenone with N,N-dimethylformamide di-Me acetal. I showed inhibition of PTP 1B with IC50 values of 0.14-80 μ M, antidiabetic effect in diet induced obese mouse model, and etc. Thus, I and their pharmaceutical compns. are useful for the treatment or prevention of PTP-1B mediated diseases, including diabetes, obesity, and diabetes-related diseases.

IT 921848-21-7P, 2-Amino-4-methylamino-7-(2-trifluoromethylphenyl)pyrido[2,3-d]pyrimidine-6-carboxylic acid trifluoroacetate

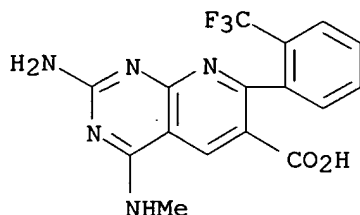
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrido[2,3-d] pyrimidine-2,4-diamine compds. as PTP1B inhibitors)

RN 921848-21-7 CAPLUS

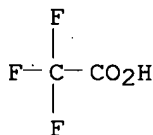
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 2-amino-4-(methylamino)-7-[2-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CRN 921848-20-6
CMF C16 H12 F3 N5 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1164714 CAPLUS

DOCUMENT NUMBER: 144:63822

TITLE: Determination of methotrexate, several pteridines, and creatinine in human urine, previous oxidation with potassium permanganate, using HPLC with photometric and fluorimetric serial detection

AUTHOR(S): Duran Meras, Isabel; Espinosa Mansilla, Anunciacion; Rodriguez Gomez, M. Jose

CORPORATE SOURCE: Department of Analytical Chemistry, University of Extremadura, Badajoz, 06071, Spain

SOURCE: Analytical Biochemistry (2005), 346(2), 201-209
CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Elsevier

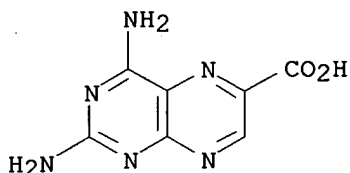
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel HPLC method, using UV and fluorimetric serial detection, for the simultaneous determination of methotrexate (MTX), five disease marker pteridines,

and the reference metabolic subproduct creatinine (CREA) in human urine was established. A previous oxidation process using 10-3 M KMnO4 (pH 5.0) and 35 min of oxidation time was necessary to transform the analytes in the highly fluorescent pteridinic rings. CREA was not affected by the oxidative medium. Using Tris-HCl/NaCl buffer solution (pH 6.6) as mobile phase, MTX and the assayed pteridines were monitored by fluorescence at $\lambda_{em} = 444$ nm and $\lambda_{ex} = 280$ nm and creatinine was monitored by absorption measurements at $\lambda_{abs} = 230$ nm. All components were well resolved in approx. 7 min. Detection limits, according the criteria of Clayton and co-workers, were 10 ng ml⁻¹ for MTX, less than 1 ng ml⁻¹ for all of the

pteridines, and 4 µg ml⁻¹ for CREA.
 IT 716-74-5
 RL: ANT (Analyte); ANST (Analytical study)
 (determination of methotrexate, several pteridines, and creatinine in human urine)
 RN 716-74-5 CAPLUS
 CN 6-Pteridinecarboxylic acid, 2,4-diamino- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:343589 CAPLUS

DOCUMENT NUMBER: 141:167199

TITLE: Design, synthesis, and computational affinity prediction of ester soft drugs as inhibitors of dihydrofolate reductase from *Pneumocystis carinii*
 AUTHOR(S): Graffner-Nordberg, Malin; Kolmodin, Karin; Aqvist, Johan; Queener, Sherry F.; Hallberg, Anders

CORPORATE SOURCE: Uppsala Biomedical Center, Department of Medicinal Chemistry, Uppsala University, Uppsala, SE-751 23, Swed.

SOURCE: European Journal of Pharmaceutical Sciences (2004), 22(1), 43-54
 CODEN: EPSCED; ISSN: 0928-0987

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:167199

AB A series of dihydrofolate reductase (DHFR) inhibitors, where the methylenamino-bridge of nonclassical inhibitors was replaced with an ester function, have been prepared as potential soft drugs intended for inhalation against *Pneumocystis carinii* pneumonia (PCP). Several of the new ester-based inhibitors that should serve as good substrates for the ubiquitous esterases and possibly constitute safer alternatives to metabolically stable DHFR inhibitors administered orally, were found to be potent inhibitors of *P. carinii* DHFR (pcDHFR). Although the objectives of the present program is to achieve a favorable toxicity profile by applying the soft drug concept, a high preference for inhibition of the fungal DHFR vs. the mammalian DHFR is still desirable to suppress host toxicity at the site of administration. Compds. with a slight preference for the fungal enzyme were identified. The selection of the target compds. for synthesis was partly guided by an automated docking and scoring procedure as well as mol. dynamics simulations. The modest selectivity of the synthesized inhibitors was reasonably well predicted, although a correct ranking of the relative affinities was not successful in all cases.

IT 454439-45-3P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

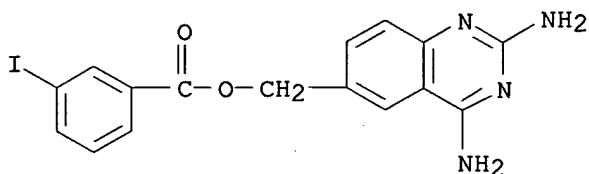
(design, synthesis, and computational affinity prediction of ester soft drugs as inhibitors of dihydrofolate reductase from *Pneumocystis*)

10/525,906

carinii)

RN 454439-45-3 CAPLUS

CN Benzoic acid, 3-iodo-, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



IT 454439-27-1P 454439-29-3P 454439-31-7P

454439-33-9P 454439-35-1P 454439-37-3P

454439-38-4P 454439-39-5P 454439-40-8P

454439-41-9P 454439-42-0P 454439-43-1P

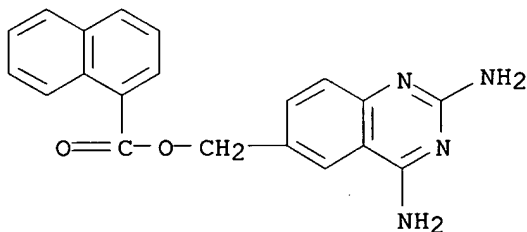
454439-44-2P 454439-46-4P 735334-45-9P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and computational affinity prediction of ester soft drugs as inhibitors of dihydrofolate reductase from *Pneumocystis carinii*)

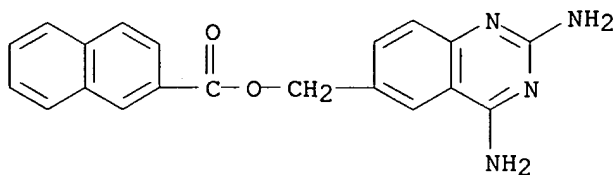
RN 454439-27-1 CAPLUS

CN 1-Naphthalenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



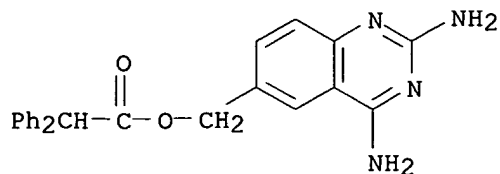
RN 454439-29-3 CAPLUS

CN 2-Naphthalenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



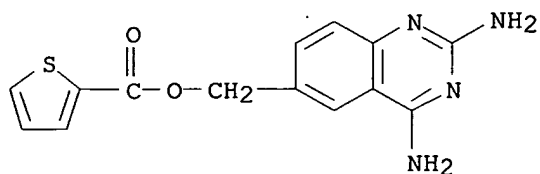
RN 454439-31-7 CAPLUS

CN Benzeneacetic acid, α -phenyl-, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



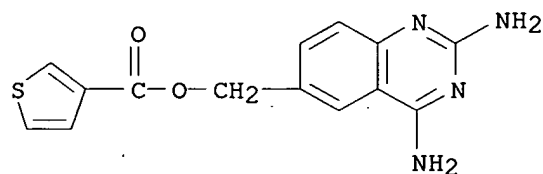
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CN 2-Thiophenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



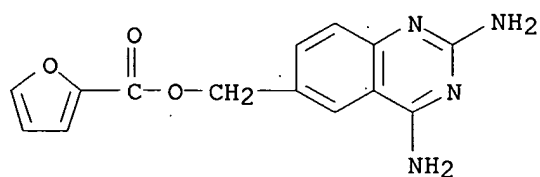
RN 454439-35-1 CAPLUS

CN 3-Thiophenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



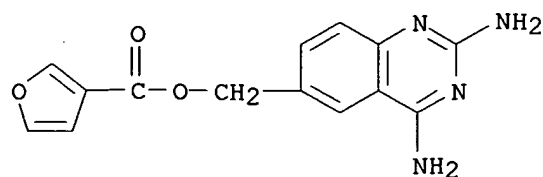
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CN 2-Furancarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



RN 454439-38-4 CAPLUS

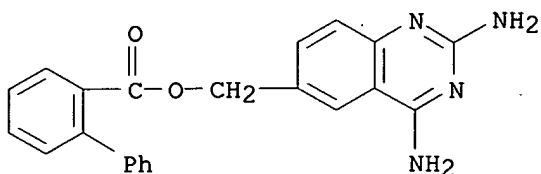
CN 3-Furancarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



10/525,906

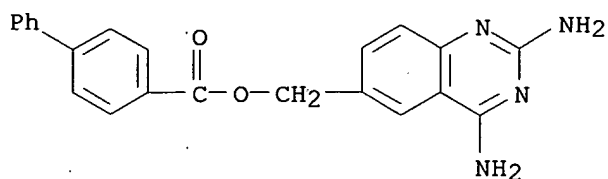
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CN [1,1'-Biphenyl]-2-carboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



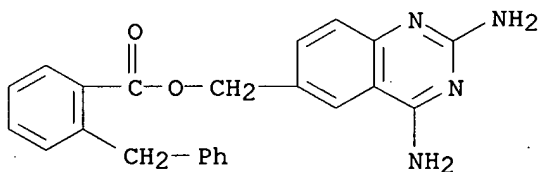
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CN [1,1'-Biphenyl]-4-carboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



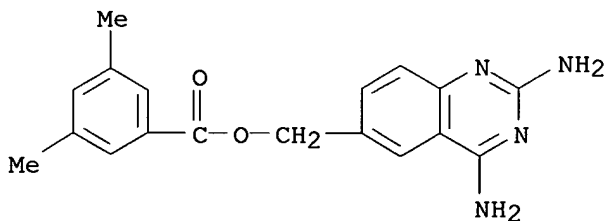
RN 454439-41-9 CAPLUS

CN Benzoic acid, 2-(phenylmethyl)-, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



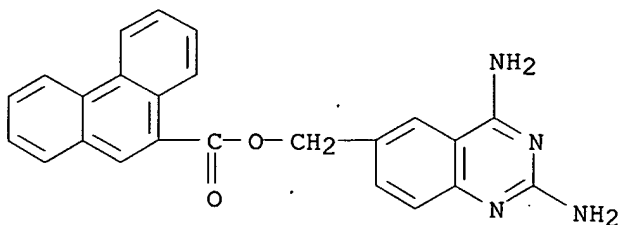
RN 454439-42-0 CAPLUS

CN Benzoic acid, 3,5-dimethyl-, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



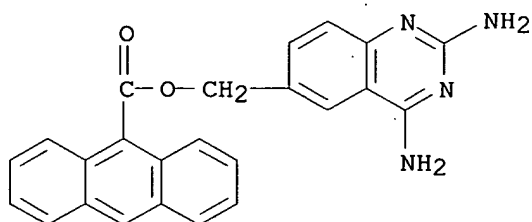
RN 454439-43-1 CAPLUS

CN 9-Phenanthrenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



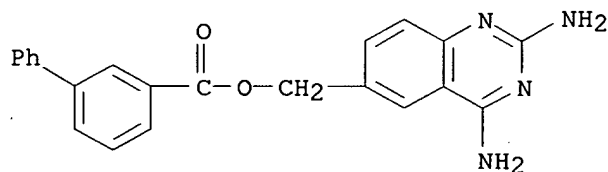
RN 454439-44-2 CAPLUS

CN 9-Anthracenecarboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



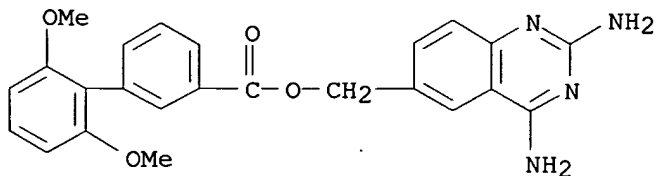
RN 454439-46-4 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



RN 735334-45-9 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2',6'-dimethoxy-, (2,4-diamino-6-quinazolinyl)methyl ester (CA INDEX NAME)



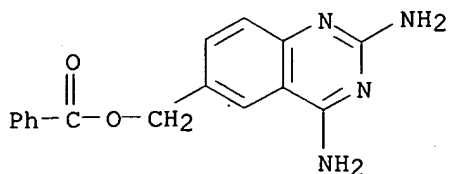
IT 206655-64-3

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(design, synthesis, and computational affinity prediction of ester soft drugs as inhibitors of dihydrofolate reductase from *Pneumocystis carinii*)

RN 206655-64-3 CAPLUS

CN 6-Quinazolinemethanol, 2,4-diamino-, 6-benzoate (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:566419 CAPLUS

DOCUMENT NUMBER: 133:271778

TITLE: Densitometric determination of impurities in pharmaceuticals part V. Determination of folic acid and 2,4-diaminopteridine-6-carboxylic acid in methotrexate

AUTHOR(S): Krzek, Jan; Kwiecien, Anna

CORPORATE SOURCE: Department of Inorganic and Analytical Chemistry, Collegium Medicum, Krakow, 30-688, Pol.

SOURCE: Chemia Analityczna (Warsaw) (2000), 45(4), 551-559
CODEN: CANWAJ; ISSN: 0009-2223

PUBLISHER: Institute of Physical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A chromatog. and densitometric method has been developed for the identification and quant. determination of folic acid and

2,4-diaminopteridine-6-carboxylic acid occurring as impurities in methotrexate. Two mobile phases were used for the separation: glacial acetic acid-dimethylsulfoxide-propanol-2-ammonia 25% (2:8:25:5 volume/volume) and dimethylsulfoxide-propanol-2-ammonia 25% (7:30:8 volume/volume) and ready to use HPTLC plates as stationary phase. Detection was carried out directly on plates together with quant. densitometric measurements in UV at $\lambda = 273$ nm and fluorimetric at $\lambda = 366$ nm. The newly developed method appears to be useful for the direct determination of folic acid

and 2,4-diaminopteridine-6-carboxylic acid. Statistical anal. has proved that this method is accurate and repeatable.

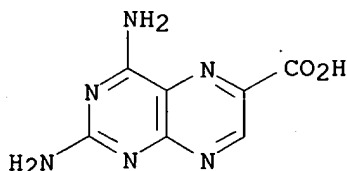
IT 716-74-5, 2,4-Diaminopteridine-6-carboxylic acid

RL: ANT (Analyte); ANST (Analytical study)

(determination of folic acid and diaminopteridinecarboxylic acid in methotrexate)

RN 716-74-5 CAPLUS

CN 6-Pteridinecarboxylic acid, 2,4-diamino- (CA INDEX NAME)



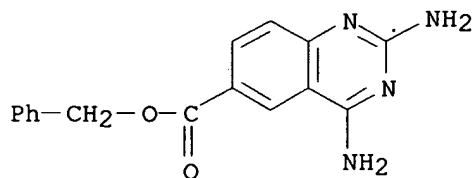
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

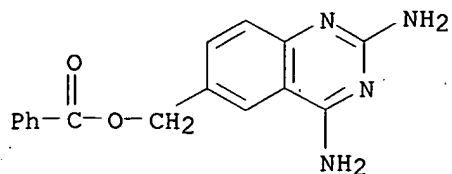
ACCESSION NUMBER: 1998:278507 CAPLUS
DOCUMENT NUMBER: 129:4621
ORIGINAL REFERENCE NO.: 129:1109a,1112a
TITLE: Synthesis and enzymic hydrolysis of esters,
constituting simple models of soft drugs
AUTHOR(S): Graffner-Nordberg, Malin; Sjodin, Karin; Tunek,
Anders; Hallberg, Anders
CORPORATE SOURCE: Dep. Organic Pharm. Chem., Uppsala Biomed. Cent.,
Uppsala Univ., Uppsala, SE-751 23, Swed.
SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(4),
591-601
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:4621

AB One way to minimize systemic side effects of drugs is to design mols., soft drugs, in such a way that they are metabolically inactivated rapidly after having acted on their pharmacol. target. Hydrolases (esterases, peptidases, lipases, glycosidases, etc.) are enzymes well suited to use for drug inactivation since they are ubiquitously distributed. Insertion of ester bonds susceptible to enzymic cleavage may represent one approach to make the action of a drug more restricted to the site of application. The present study describes the chemical synthesis of fourteen model compds. comprising a bicyclic aromatic unit connected by an ester-containing bridge to another aromatic ring. Initial attempts to define (a) the tissue selectivity of the hydrolytic metabolism and (b) the mol. structural factors affecting the rate of enzymic ester cleavage are presented. The data show that human and rat liver fractions were more active than human duodenal mucosa and human blood leukocytes at hydrolyzing the compds. The rank order of the compds. was, however, very similar in the different biol. systems. Com. available pig liver carboxyl and cholesterol esterase both reasonably well predict the rank order in the tissue fractions.

IT 206655-63-2P 206655-64-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and enzymic hydrolysis of esters, constituting simple models of soft drugs)
RN 206655-63-2 CAPLUS
CN 6-Quinazolinecarboxylic acid, 2,4-diamino-, phenylmethyl ester (CA INDEX NAME)



RN 206655-64-3 CAPLUS
CN 6-Quinazolinemethanol, 2,4-diamino-, 6-benzoate (CA INDEX NAME)



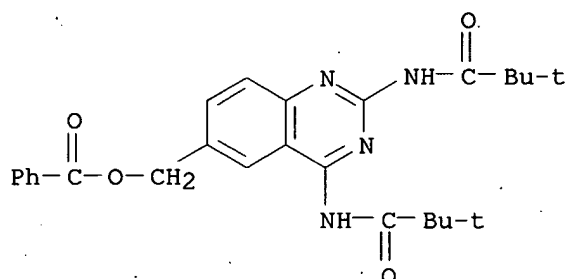
IT 206655-66-5P 206655-68-7P 206655-75-6P
207562-23-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and enzymic hydrolysis of esters, constituting simple models of soft drugs)

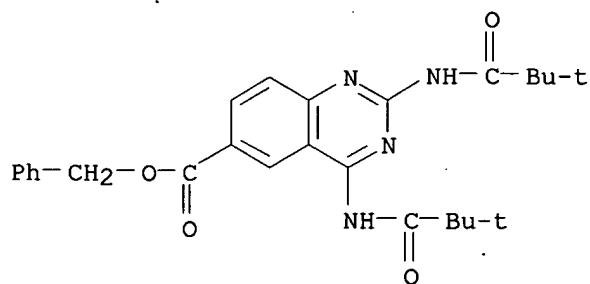
RN 206655-66-5 CAPLUS

CN Propanamide, N,N'-[6-[(benzyloxy)methyl]-2,4-quinazolinediyl]bis[2,2-dimethyl- (9CI) (CA INDEX NAME)



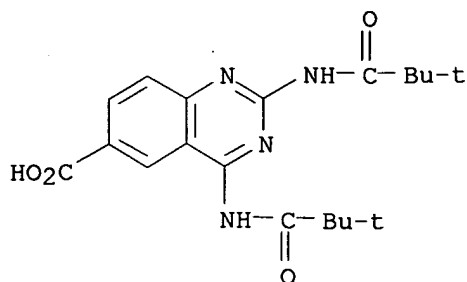
RN 206655-68-7 CAPLUS

CN 6-Quinazolinecarboxylic acid, 2,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-, phenylmethyl ester (CA INDEX NAME)



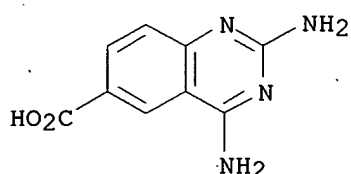
RN 206655-75-6 CAPLUS

CN 6-Quinazolinecarboxylic acid, 2,4-bis[(2,2-dimethyl-1-oxopropyl)amino]- (CA INDEX NAME)



RN 207562-23-0 CAPLUS

CN 6-Quinazolinecarboxylic acid, 2,4-diamino- (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:224587 CAPLUS

DOCUMENT NUMBER: 128:303635

ORIGINAL REFERENCE NO.: 128:60001a,60004a

TITLE: Enzymic hydrolysis of soft drug models of antifolates

AUTHOR(S): Graffner-Nordberg, M.; Sjodin, K.; Tunek, A.; Hellberg, A.

CORPORATE SOURCE: Department of Organic Pharmaceutical Chemistry, Uppsala Biomedical Centre, Uppsala University, Swed.

SOURCE: Chemistry and Biology of Pteridines and Folates 1997, Proceedings of the International Symposium on Pteridines and Folates, 11th, Berchtesgaden, Germany, June 15-20, 1997 (1997), 225-228. Editor(s): Pfleiderer, Wolfgang; Rokos, Hartmut. Blackwell Wissenschafts-Verlag GmbH: Berlin, Germany.

CODEN: 65VBAF

DOCUMENT TYPE: Conference

LANGUAGE: English

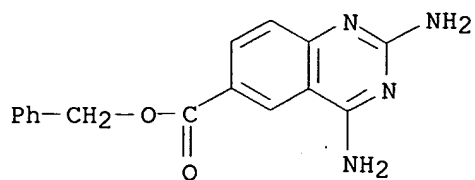
AB In the study, a comparison is presented of the rates of hydrolysis of some soft drugs by pig liver carboxyl esterase and/or cholesterol esterase from pancreas, liver, duodenum, and leukocytes.

IT 206655-63-2P 206655-64-3P

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC- (Process); USES (Uses) (enzymic hydrolysis of soft drug models of antifolates)

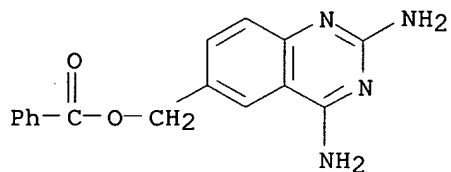
RN 206655-63-2 CAPLUS

CN 6-Quinazolinecarboxylic acid, 2,4-diamino-, phenylmethyl ester (CA INDEX NAME)



RN 206655-64-3 CAPLUS

CN 6-Quinazolinemethanol, 2,4-diamino-, 6-benzoate (CA INDEX NAME)



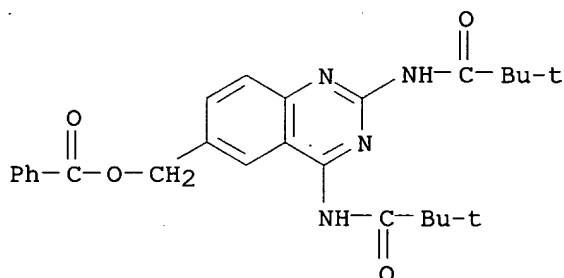
IT 206655-66-5P 206655-68-7P 206655-75-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(enzymic hydrolysis of soft drug models of antifolates)

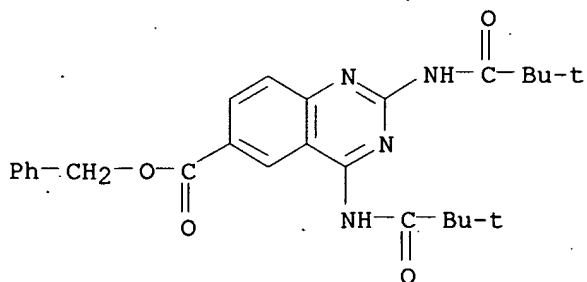
RN 206655-66-5 CAPLUS

CN Propanamide, N,N'-[6-[(benzoyloxy)methyl]-2,4-quinazolinediyl]bis[2,2-dimethyl- (9CI) (CA INDEX NAME)



RN 206655-68-7 CAPLUS

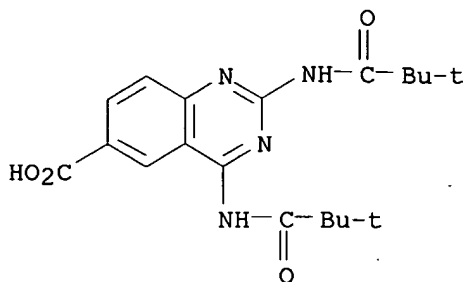
CN 6-Quinazolinecarboxylic acid, 2,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-, phenylmethyl ester (CA INDEX NAME)



RN 206655-75-6 CAPLUS

CN 6-Quinazolinecarboxylic acid, 2,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-

(CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:33977 CAPLUS

DOCUMENT NUMBER: 126:54463

ORIGINAL REFERENCE NO.: 126:10583a,10586a

TITLE: Analogs of Methotrexate in Rheumatoid Arthritis. 1. Effects of 10-Deazaaminopterin Analogs on Type II Collagen-Induced Arthritis in Mice

AUTHOR(S): DeGraw, Joseph I.; Colwell, William T.; Crase, Jac; Smith, R. Lane; Piper, James R.; Waud, William R.; Sirotnak, Francis M.

CORPORATE SOURCE: Bio-Organic Chemistry Laboratory, SRI International, Menlo Park, CA, 94025, USA

SOURCE: Journal of Medicinal Chemistry (1997), 40(3), 370-376
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Carbonation of the dianions (LDA) of 5-methylthiophene-2-carboxylic, 2-methylpyridine-5-carboxylic, and 3-methylpyridine-6-carboxylic acids provided the resp. carboxy heteroarylacetic acids. The crude diacids were directly esterified in MeOH-HCl to afford the diesters. Alkylation of the sodio anions with Et iodide yielded the appropriate α -Et diesters. The anions of the various diester substrates were then alkylated by 2,4-diamino-6-(bromomethyl)pteridine followed by ester saponification at room temperature to afford

the resp. 2,4-diamino-4-deoxy-10-carboxy-10-deazapteroic acids. The 10-carboxyl group was readily decarboxylated by heating in DMSO at temps. of 110-135 °C to give the diamino 10-deaza heteropteroid acid intermediates. Coupling with di-Et L-glutamate followed by ester hydrolysis afforded the target aminopterins. The analogs were evaluated for antiinflammatory effect in the mouse type II collagen model. The thiophene analog of 10-ethyl-10-deazaaminopterin was found to be an effective inhibitor in terms of reduced visual evidence of inflammation and swelling as determined by caliper measurement.

IT 153802-50-7P 153802-51-8P 154586-65-9P

154586-66-0P 154586-71-7P 154586-75-1P

154586-76-2P 154586-81-9P 154586-83-1P

154586-87-5P

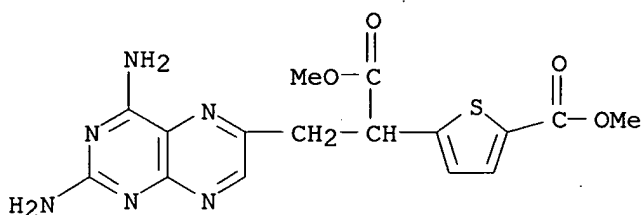
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation and antiarthritic activity of 10-deazaaminopterin analogs)

10/525,906

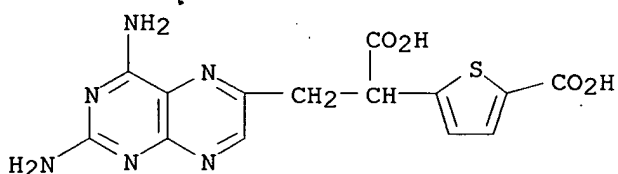
RN 153802-50-7 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



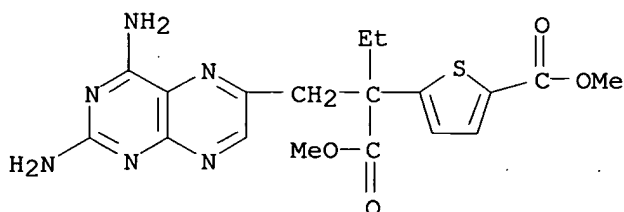
RN 153802-51-8 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-thienyl)- (CA INDEX NAME)



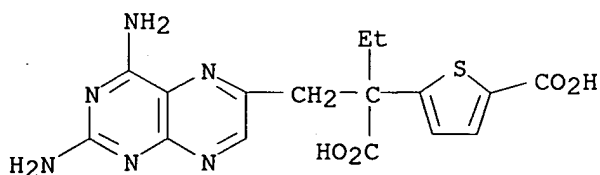
RN 154586-65-9 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -ethyl- α -[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



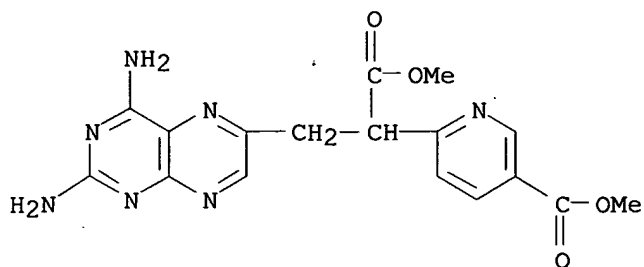
RN 154586-66-0 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-thienyl)- α -ethyl- (CA INDEX NAME)



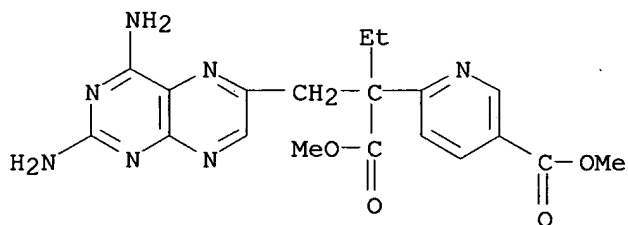
RN 154586-71-7 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[5-(methoxycarbonyl)-2-pyridinyl]-, methyl ester (CA INDEX NAME)



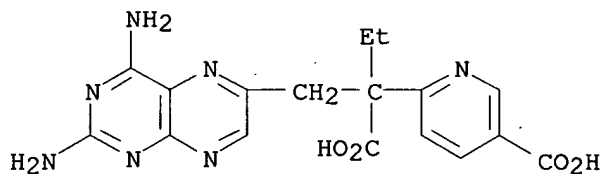
RN 154586-75-1 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-ethyl-α-[5-(methoxycarbonyl)-2-pyridinyl]-, methyl ester (CA INDEX NAME)



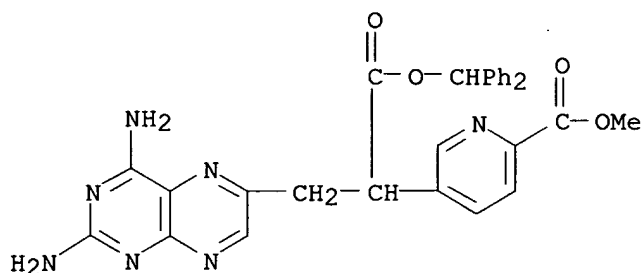
RN 154586-76-2 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-(5-carboxy-2-pyridinyl)-α-ethyl- (CA INDEX NAME)



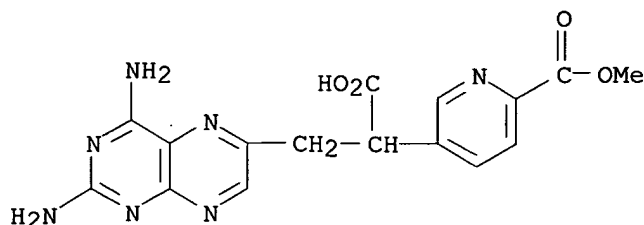
RN 154586-81-9 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-[6-(methoxycarbonyl)-3-pyridinyl]-, diphenylmethyl ester (CA INDEX NAME)

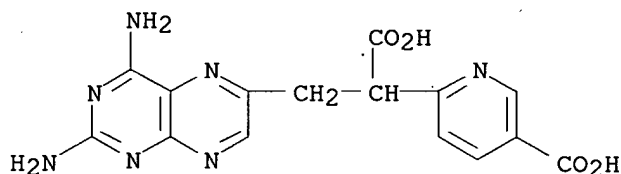


RN 154586-83-1 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-[6-(methoxycarbonyl)-3-pyridinyl]- (CA INDEX NAME)



RN 154586-87-5 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-(5-carboxy-2-pyridinyl)-
(CA INDEX NAME)REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:483913 CAPLUS

DOCUMENT NUMBER: 125:196375

ORIGINAL REFERENCE NO.: 125:36799a,36802a

TITLE: Preparation of [(diaminopyridopyrimidinyl)methylamino
]benzoyl]glutamates and analogs as antiinflammatory
and antineoplastic agentsINVENTOR(S): Degraw, Joseph I.; Colwell, William T.; Sirotnak,
Francis M.; Smith, R. Lane; Piper, James R.

PATENT ASSIGNEE(S): Sri International, USA; Sloan-Kettering Institute

SOURCE: U.S., 31 pp., Cont.-in-part of U.S. 5,354,751.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

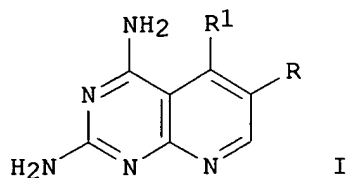
FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5536724	A	19960716	US 1993-140793	19931021
US 5374726	A	19941220	US 1993-28431	19930309
US 5354751	A	19941011	US 1993-90750	19930712
PRIORITY APPLN. INFO.:			US 1992-845407	B2 19920303
			US 1992-875779	B2 19920429
			US 1992-938105	B2 19920831
			US 1993-8919	B2 19930126
			US 1993-28431	A2 19930309
			US 1993-90750	A2 19930712

OTHER SOURCE(S): MARPAT 125:196375

GI



AB Title compds. [I; R = CH₂Z₁Z₂CONHCH(CO₂H)CH₂CH₂CO₂H; R₁ = H or alkyl; Z₁ = CHR₂, NR₂; R₂ = H, alk(en)yl, alkynyl; Z₂ = 1,4-phenylene, 2,5-thienylene, pyridine-2,5-diyl, etc.] were prepared. Thus, PrC(OMe)₃ was cyclocondensed with 2 CH₂(CN)₂ and the dechlorinated product cyclocondensed with guanidine to give I (R₁ = Pr) (II; R = cyano) which was reductively condensed with L-4-(H₂N)C₆H₄CONHCH(CO₂H)CH₂CH₂CO₂H to give II [R = L-CH₂NH₂Z₂CONHCH(CO₂H)CH₂CH₂CO₂H, Z₂ = 1,4-phenylene]. Data for antiinflammatory and antineoplastic activity of I were given.

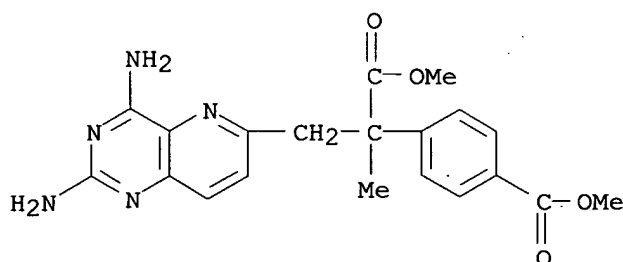
IT 88392-94-3P 146464-91-7P 146464-92-8P
 153802-45-0P 153802-46-1P 153802-48-3P
 153802-50-7P 153802-51-8P 153802-54-1P
 153802-55-2P 153802-57-4P 153802-86-9P
 153802-88-1P 153802-92-7P 153802-93-8P
 180634-15-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [[(diaminopyridopyrimidinyl)methylamino]benzoyl]glutamates and analogs as antiinflammatory and antineoplastic agents).

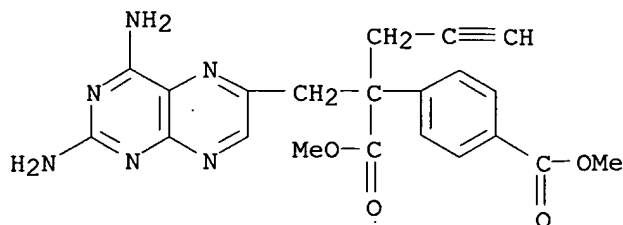
RN 88392-94-3 CAPLUS

CN Pyrido[3,2-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-[4-(methoxycarbonyl)phenyl]-α-methyl-, methyl ester (CA INDEX NAME)



RN 146464-91-7 CAPLUS

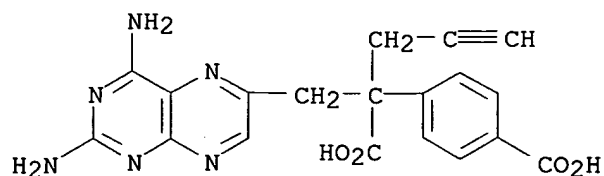
CN 6-Pteridinepropanoic acid, 2,4-diamino-α-[4-(methoxycarbonyl)phenyl]-α-2-propyn-1-yl-, methyl ester (CA INDEX NAME)



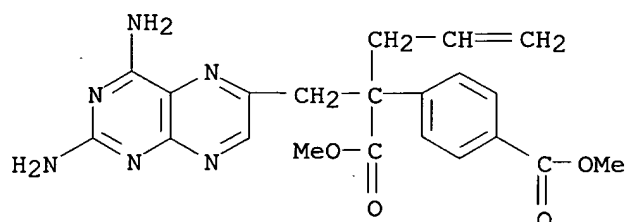
RN 146464-92-8 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-(4-carboxyphenyl)-α-2-

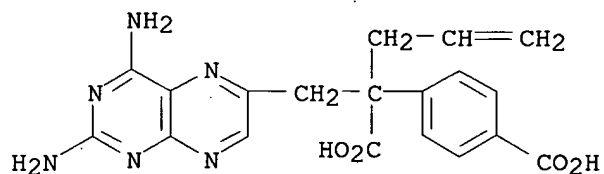
propyn-1-yl- (CA INDEX NAME)



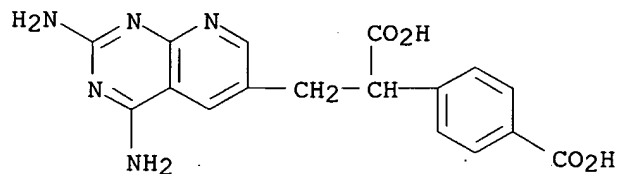
RN 153802-45-0 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[4-(methoxycarbonyl)phenyl]- α -2-propen-1-yl-, methyl ester (CA INDEX NAME)

RN 153802-46-1 CAPLUS

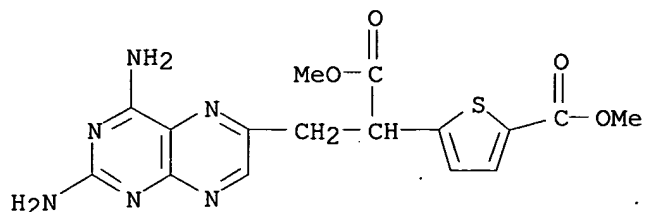
CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(4-carboxyphenyl)- α -2-propen-1-yl- (CA INDEX NAME)

RN 153802-48-3 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino- α -(4-carboxyphenyl)- (CA INDEX NAME)

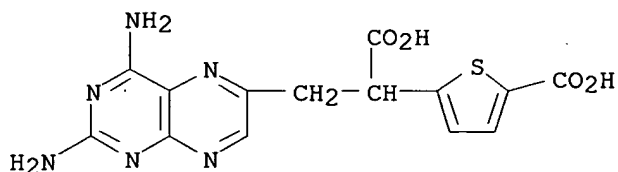
RN 153802-50-7 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



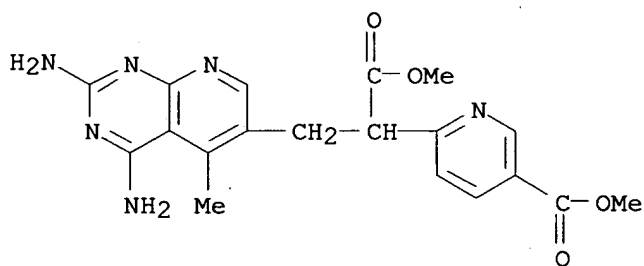
RN 153802-51-8 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino-α-(5-carboxy-2-thienyl)- (CA INDEX NAME)



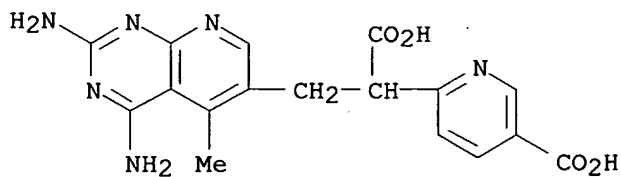
RN 153802-54-1 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-[5-(methoxycarbonyl)-2-pyridinyl]-5-methyl-, methyl ester (CA INDEX NAME)



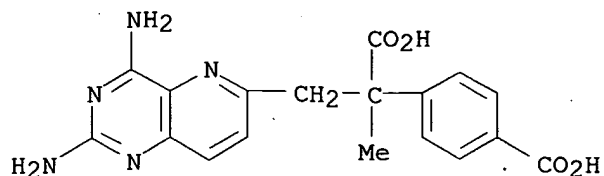
RN 153802-55-2 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-(5-carboxy-2-pyridinyl)-5-methyl- (CA INDEX NAME)



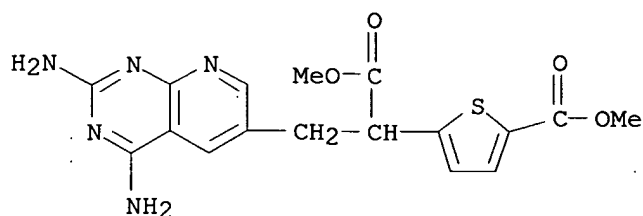
RN 153802-57-4 CAPLUS

CN Pyrido[3,2-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-(4-carboxyphenyl)-α-methyl- (CA INDEX NAME)



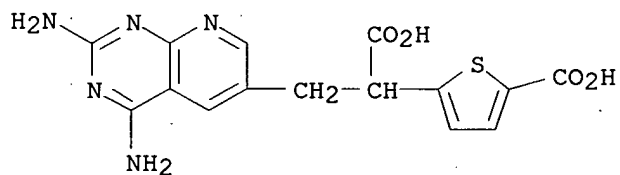
RN 153802-86-9 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



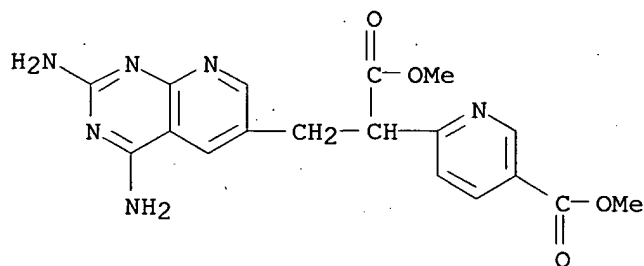
RN 153802-88-1 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-(5-carboxy-2-thienyl)- (CA INDEX NAME)



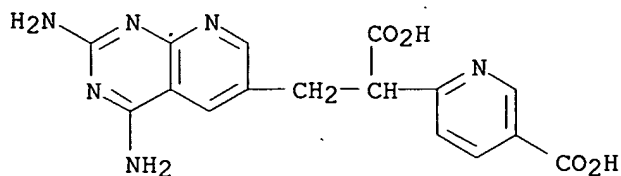
RN 153802-92-7 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-[5-(methoxycarbonyl)-2-pyridinyl]-, methyl ester (CA INDEX NAME)



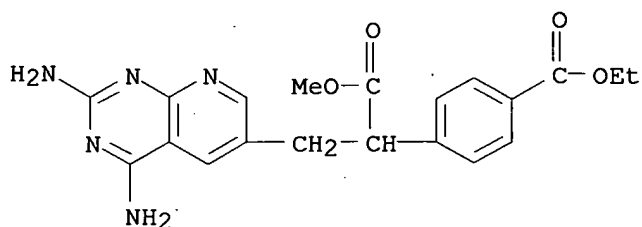
RN 153802-93-8 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-(5-carboxy-2-pyridinyl)- (CA INDEX NAME)



RN 180634-15-5 CAPLUS

CN Pyrido[2,3-d]pyrimidine-6-propanoic acid, 2,4-diamino-α-[4-(ethoxycarbonyl)phenyl]-, methyl ester (CA INDEX NAME)



L7 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:270453 CAPLUS

DOCUMENT NUMBER: 120:270453

ORIGINAL REFERENCE NO.: 120:47919a,47922a

TITLE: Heteroaroyl-10-deazaaminopterin for treatment of inflammation and arthritis

INVENTOR(S): Degraw, Joseph I.; Colwell, William T.; Sirotnak, Francis M.; Smith, R. Lane; Piper, James R.

PATENT ASSIGNEE(S): SRI International, USA

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

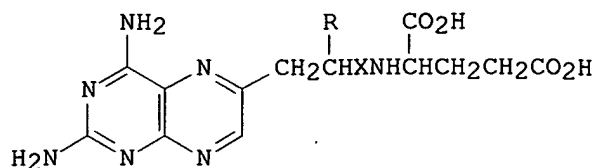
DOCUMENT TYPE: Patent

LANGUAGE: English

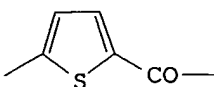
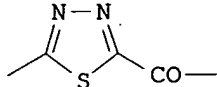
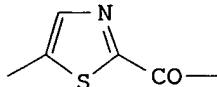
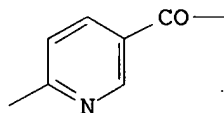
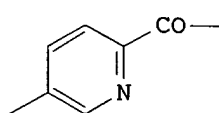
FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9322315	A1	19931111	WO 1993-US3963	19930428
W: AU, CA, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9341199	A	19931129	AU 1993-41199	19930428
PRIORITY APPLN. INFO.:			US 1992-875779	A 19920429
			US 1992-938105	A 19920831
			WO 1993-US3963	A 19930428
OTHER SOURCE(S):		MARPAT 120:270453		
GI				



I

Q¹=Q²=Q³=Q⁴=Q⁵=

AB The title compds. (I; R = H, alkyl, alkenyl, alkynyl; X = Q¹-Q⁵), useful for treating arthritis and other proliferative diseases, are prepared and I-containing formulations presented. Thus, I (R = Et, X = Q¹), which was prepared from Me 2-(carbomethoxy)thiophene-5-acetate in 6 steps, demonstrated average thickness of rear mice paws, which had been subjected to an antigenic challenge with type-II collagen, of 2.15-2.26 mm after 30-44 days, vs. 2.29-2.73 mm for untreated mice.

IT 153802-50-7 153802-51-8 154586-65-9

154586-66-0 154586-71-7 154586-75-1

154586-76-2 154586-81-9 154586-83-1

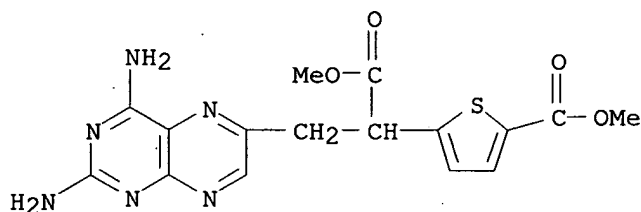
154586-87-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation as intermediate in preparation of antiinflammatory agents)

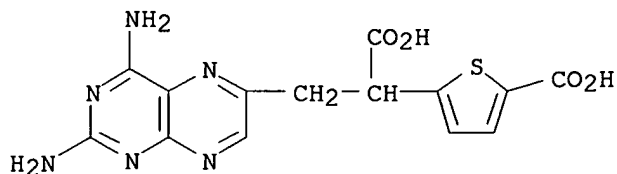
RN 153802-50-7 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



RN 153802-51-8 CAPLUS

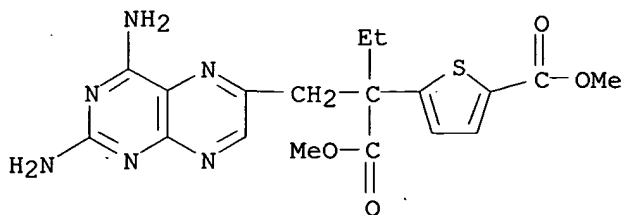
CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-thienyl)- (CA INDEX NAME)



10/525,906

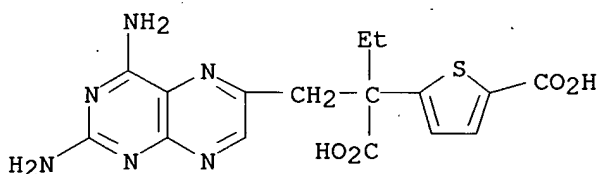
RN 154586-65-9 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -ethyl- α -[5-(methoxycarbonyl)-2-thienyl]-, methyl ester (CA INDEX NAME)



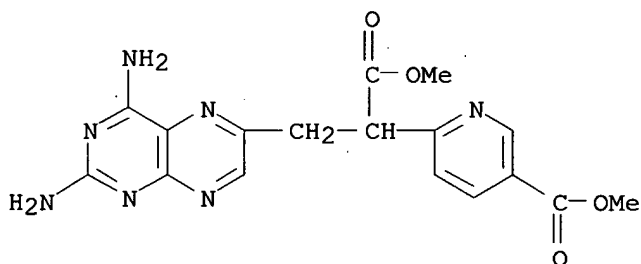
RN 154586-66-0 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-thienyl)- α -ethyl- (CA INDEX NAME)



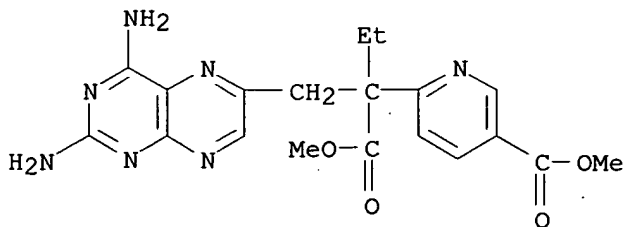
RN 154586-71-7 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[5-(methoxycarbonyl)-2-pyridinyl]-, methyl ester (CA INDEX NAME)



RN 154586-75-1 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -ethyl- α -[5-(methoxycarbonyl)-2-pyridinyl]-, methyl ester (CA INDEX NAME)

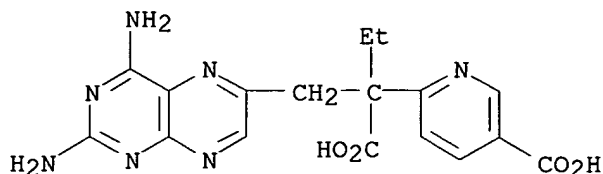


RN 154586-76-2 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-pyridinyl)-

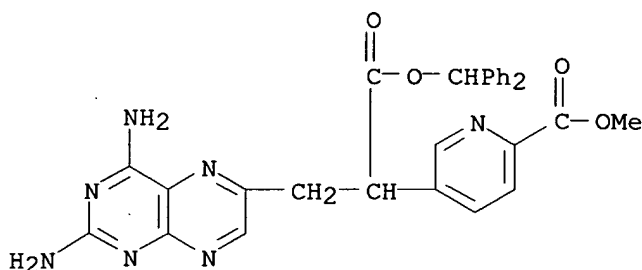
10/525,906

α -ethyl- (CA INDEX NAME)



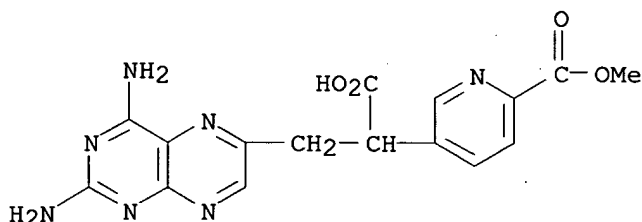
RN 154586-81-9 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[6-(methoxycarbonyl)-3-pyridinyl]-, diphenylmethyl ester (CA INDEX NAME)



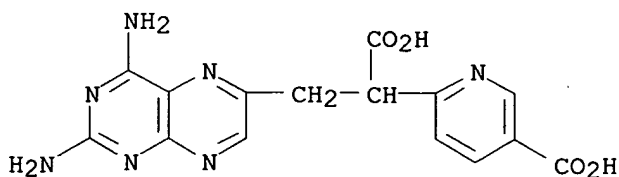
RN 154586-83-1 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -[6-(methoxycarbonyl)-3-pyridinyl]- (CA INDEX NAME)



RN 154586-87-5 CAPLUS

CN 6-Pteridinepropanoic acid, 2,4-diamino- α -(5-carboxy-2-pyridinyl)- (CA INDEX NAME)



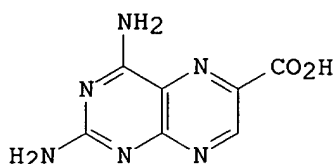
L7 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:407344 CAPLUS

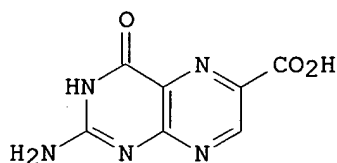
DOCUMENT NUMBER: 111:7344

ORIGINAL REFERENCE NO.: 111:1407a,1410a

TITLE: Studies on pyrazines. 17. An efficient synthesis of pteridine-6-carboxylic acids
 AUTHOR(S): Sato, Nobuhiro; Saito, Noriko
 CORPORATE SOURCE: Dep. Chem., Yokohama City Univ., Yokohama, 236, Japan
 SOURCE: Journal of Heterocyclic Chemistry (1988), 25(6), 1737-40
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 111:7344
 GI

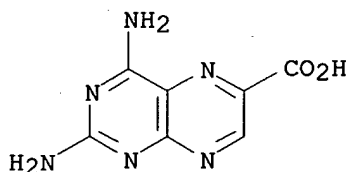


I



II

AB 2,4-Diaminopteridine-6-carboxylic acid (I) and pterin-6-carboxylic acid (II) were prepared by permanganate oxidation of the corresponding 6-(2-furyl)-substituted pteridines under mild conditions. Several attempts to cleave the furan ring with other oxidizing agents are also described.
 IT 716-74-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and alkaline hydrolysis of, pterincarboxylic acid from)
 RN 716-74-5 CAPLUS
 CN 6-Pteridinecarboxylic acid, 2,4-diamino- (CA INDEX NAME)



L7 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1973:432274 CAPLUS
 DOCUMENT NUMBER: 79:32274
 ORIGINAL REFERENCE NO.: 79:5249a,5252a
 TITLE: Synthesis of pteridine-6-carboxamides. 9-Oxofolic acid and 9-oxoaminopterin
 AUTHOR(S): Nair, M. G.; Baugh, Charles M.
 CORPORATE SOURCE: Nutr. Program, Univ. Alabama, Birmingham, AL, USA
 SOURCE: Journal of Organic Chemistry (1973), 38(12), 2185-9
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new method for the preparation of several 7-unsubstituted pteridine-6-carboxamides is reported. This method was used for the synthesis of 9-oxofolic acid and 9-oxoaminopterin as well as

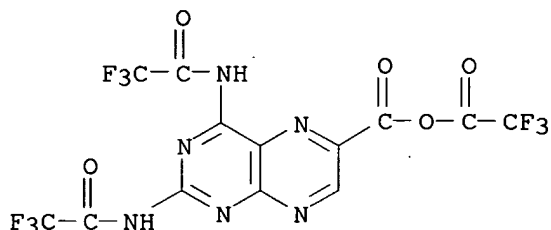
γ -glutamyl derivs. These procedures utilize the mixed anhydride of a pteridine-6-carboxylic acid with F₃CCO₂H. The activated pteridines are stable enough to permit removal of excess (F₃CCO)₂O and F₃CCO₂H followed by direct coupling to nucleophiles such as amines and amino acids. The preparation of α -amino-p-toluic acid is also reported.

IT 39707-67-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amino acids)

RN 39707-67-0 CAPLUS

CN 6-Pteridinecarboxylic acid, 2,4-bis[(trifluoroacetyl)amino]-, anhydride with trifluoroacetic acid (9CI) (CA INDEX NAME)



L7 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:403560 CAPLUS

DOCUMENT NUMBER: 75:3560

ORIGINAL REFERENCE NO.: 75:591a,594a

TITLE: Mode of action of pteridine diuretics. II.
Degradation of 2,4-diamino-6,7-dimethylpteridine and simultaneous inhibition of uric acid excretion

AUTHOR(S): Eder, J.; Rembold, H.

CORPORATE SOURCE: Max-Planck-Inst. Biochem., Munich, Fed. Rep. Ger.

SOURCE: Arzneimittel-Forschung (1971), 21(4), 562-5

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

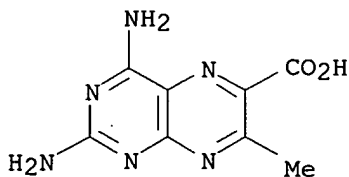
AB 2,4-Diamino-6,7-dimethylpteridine (I) fed to rats was degraded to 2,4-diamino-6-hydroxymethyl-7-methylpteridine (II) and 2,4-diamino-7-methylpteridine-6-carboxylic acid (III) which were excreted in the urine in a ratio of 3:2, and concurrently with the degradation was an 80% decrease in uric acid excretion. However, the serum uric acid remained unchanged. After feeding II to rats, 20% was excreted in the urine unchanged and 5% was oxidized to III. The diuretic activity and uric acid effect of II were somewhat less than those of I.

IT 19173-22-9

RL: FORM (Formation, nonpreparative)
(formation of, from diaminodimethylpteridine)

RN 19173-22-9 CAPLUS

CN 6-Pteridinecarboxylic acid, 2,4-diamino-7-methyl- (CA INDEX NAME)



L7 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:452105 CAPLUS

DOCUMENT NUMBER: 69:52105

ORIGINAL REFERENCE NO.: 69:9735a,9738a

TITLE: Mechanism of action of pteridine diuretics. I.
Inactivation of 2,4-diamino-6,7-dimethylpteridine and
its effects on uric acid excretion

AUTHOR(S): Eder, Joerg; Rembold, Heinz

CORPORATE SOURCE: Max-Planck-Inst. Biochem., Munich, Fed. Rep. Ger.

SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1968),
237(1), 50-9

CODEN: ZACFAU; ISSN: 0016-1152

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

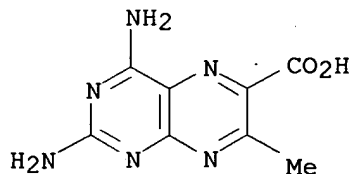
AB 2,4,6-Triaminopyrimidine, treated in aqueous solution with NaNO₂ and dilute HCl yielded the 5-nitroso derivative (I). Hydrogenation of I (Raney Ni) gave 2,4,5,6-tetraminopyrimidine (II), which crystallized from H₂O as yellow needles. The condensation product of II sulfate with biacetyl [Mallette, et al. (1947)] was purified by chromatog. over phosphocellulose [Rembold and Eder, (1967)] giving 2,4-diamino-6,7-dimethylpteridine (III). To a stirred solution containing 0.155 g. Na in 40 cc. HOCH₂CH₂OEt and 1 g. II was added dropwise with stirring, 10 cc. AcCH₂CO₂Et and the mixture refluxed 2 hrs. and worked up to give 2,4-diamino-7-methylpteridine-6-carboxylic acid (IV) as white crystals from H₂O. The isomeric 2,4-diamino-6-methyl-7-carboxylic acid (yellow crystals) was similarly prepared from II and α-oxobutyric acid. IV was converted to its Me ester by stirring in MeOH-HCl (1%) at room temperature in the dark 12 hrs. After collecting normal urine from 140-180 g. female Sprague-Dawley rats for 2 days, the animals were given 150 mg./kg. III. Urine secretion was then 3-4 times the normal amount. Comparative chromatog. (Dowex 1 + 8) of the 2 urines showed that the administered III did not appear in the urine. Repeated rechromatog. of appropriate fractions gave a purified metabolic product, which was identified by uv, N.M.R., and mass spectroscopy, and by comparison with the authentic synthetic sample as IV. In addition to the appearance of the metabolite there was a large decrease in uric acid excretion. IV had no diuretic activity and no effect on uric acid excretion. 24 references.

IT 19173-22-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19173-22-9 CAPLUS

CN 6-Pteridinecarboxylic acid, 2,4-diamino-7-methyl- (CA INDEX NAME)



L7 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:24233 CAPLUS

DOCUMENT NUMBER: 50:24233

ORIGINAL REFERENCE NO.: 50:4978d-g

TITLE: Synthesis of compounds with potential antifolic acid
activity. V. 4,7-Diamino- and 2,4,7-triaminopteridine

and its derivatives

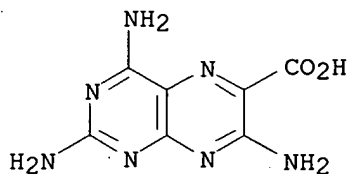
AUTHOR(S): Osdene, T. S.; Timmis, G. M.
 CORPORATE SOURCE: Roy. Cancer Hosp., London
 SOURCE: Journal of the Chemical Society (1955) 2036-8
 CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Unequivocal syntheses of 4,7-diamino- (I), 2,4,7-triamino- (II), and 4,7-diamino-2-methylthiopteridine-6-carboxylic acids (III), and their resp. carboxamides (IV, V, and VI) were prepared from 4,6-diamino- (VII), 2,4,6-triamino- (VIII), and 4,6-diamino-2-methylthio-5-nitrosopyrimidines (IX) with NCCH₂CO₂H (X) and NCCH₂CONH₂ (XI). I and II were decarboxylated to give 4,7-diamino- (XII) and 2,4,7-triaminopteridine (XIII), resp. Na alkoxides were good condensation catalysts. VII (3.2 g.) and 2 g. X were refluxed 15 min. with Na in EtOCH₂CH₂OH to yield 2.1 g. I, plates, m. 292° (effervescence), λ_{maximum} (all values taken in 4.5% HCO₂H) 269 and 369 mμ (ε 21,400 and 11,300), λ_{min}. 302 mμ (ε 2000). I (1 g.) refluxed 1 hr. with quinoline gave XII, yellow needles, m. above 300°, λ_{maximum} 255, 285, 343 mμ (ε 14,800, 4,400, and 12,500), λ_{min}. 272 and 300 mμ (ε 3800 and 3800). VII (0.7 g.) and 0.85 g. XI refluxed 2 min. in Na and EtOCH₂CH₂OH gave 0.87 g. IV, needles, m. above 300°, λ_{maximum} 271 and 374 mμ (ε 22,700 and 10,600), λ_{min}. 304 mμ (ε 1500). VIII (4.62 g.) and 2.8 g. X similarly refluxed 2.5 hrs. with Na in EtOCH₂CH₂OH gave II, needles, m. above 300°. II (1 g.) refluxed 7 hrs. in quinoline with Cu bronze gave 0.24 g. XIII, needles, m. above 300°. VIII (3 g.) and 1.8 g. XI similarly yielded 2.1 g. V, m. above 300°; triacetyl derivative (from aqueous HCONMe₂). IX (1.84 g.) and 1 g. X similarly gave III, yellow needles, m. above 300°. IX (0.9 g.) and 0.5 g. XI yielded VI as needles, m. above 300°; diacetyl derivative (from HCONMe₂).

IT 19167-55-6P, 6-Pteridinecarboxylic acid, 2,4,7-triamino-
 RL: PREP (Preparation)
 (preparation of)

RN 19167-55-6 CAPLUS
 CN 6-Pteridinecarboxylic acid, 2,4,7-triamino- (CA INDEX NAME)



L7 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:64876 CAPLUS
 DOCUMENT NUMBER: 49:64876
 ORIGINAL REFERENCE NO.: 49:12492g-i
 TITLE: Synthesis of 2,4-diamino-7-hydroxypteridine and its 6-carboxylic acid

AUTHOR(S): Osdene, T. S.; Timmis, G. M.
 CORPORATE SOURCE: Roy. Cancer Hosp., London
 SOURCE: Journal of the Chemical Society (1955) 2038-9
 CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

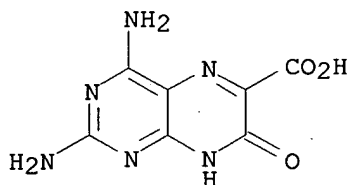
AB 2,4,6-Triamino-5-nitrosopyrimidine (3.1 g.) and CH₂(CO₂Et)₂ (25 ml.) were added to 1 g. Na dissolved in 200 ml. EtO(CH₂)₂OH, the mixture refluxed 4

hrs., cooled, the yellow solid isolated by filtration and the filtrate concentrated to dryness to yield more solid. The combined solid was purified by dissolving in boiling aqueous 2N Na₂CO₃ and filtering into boiling aqueous 2N HCl to yield 2.5 g. 2,4-diamino-7-hydroxypteridine-6-carboxylic acid (I), m. 360°. The absorption spectrum of I in 0.1N NaOH showed maximum at 350 (ϵ 14900), 260 (ϵ 11300) and 226 m μ (ϵ 38000). I (0.4 g.) sublimed at 340-60°/0.05 mm. gave 0.25 g. of pale yellow sublimate which was dissolved in dilute NH₄OH, filtered, boiled to remove NH₃, and cooled to yield 2,4-diamino-7-hydroxypteridine (II), m. above 300°. II in 0.1N NaOH showed maximum at 341 (ϵ 14100), 255 (ϵ 10900) and 224 m μ (ϵ 40300).

IT 2521-97-3P, 6-Pteridinecarboxylic acid, 2,4-diamino-7-hydroxy-
RL: PREP (Preparation)
(preparation of)

RN 2521-97-3 CAPLUS

CN 6-Pteridinecarboxylic acid, 2,4-diamino-1,7-dihydro-7-oxo- (9CI) (CA INDEX NAME)



L7 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:34968 CAPLUS

DOCUMENT NUMBER: 47:34968

ORIGINAL REFERENCE NO.: 47:5944f-i,5945a-g

TITLE: The identification of " β -dihydroxanthopterin" as 2,4-diamino-6-hydroxy-p-oxazino[2,3-d]pyrimidine

AUTHOR(S): Elion, Gertrude B.; Hitchings, George H.

CORPORATE SOURCE: Wellcome Research Labs., Tuckahoe, NY

SOURCE: Journal of the American Chemical Society (1952), 74, 3877-82

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The β -dihydroxanthopterin obtained previously by the cyclization of 5-chloroacetamido-2,4-diamino-6-pyrimidol (cf. C.A. 43, 3425h) was identified as 2,4-diamino-5H-p-oxazino[2,3-d]pyrimidin-6-ol (I). 2-Amino-4-chloro-6-pyrimidol (3 g.) and 6 g. H₂NCH₂CO₂Et.HCl were heated 1 hr. at 135° and then 1.5 hrs. at 135° the mixture was extracted with EtOH, Et₂O added, the precipitate leached with cold Me₂CO, and the residue extracted with 20 cc. H₂O to give a solution of 600-700 mg. 2-amino-4-carboxymethylamino-6-hydroxypyrimidine (II), λ_{maximum} 268 m μ , O.D. 0.5.5 (at pH 1), 268 m μ , O.D. 0.47 (at pH 11) [2,4-diamino-6-pyrimidol, λ_{maximum} 265 m μ , E_{max}. 20000 (at pH 1), 265 m μ , E_{max}. 12500 (at pH 11); 2-amino-4-chloropyrimidinol, λ_{maximum} 286 m μ (at pH 1); 275 m μ (at pH 11)]. The aqueous solution of II and 0.35 g. diazotized p-ClC₆H₄NH₂ at pH 5 gave 0.35 g. yellow azo compound, which, dissolved in 50% boiling EtOH and refluxed 5 min. with 750 mg. Zn dust and 1 cc. 6 N H₂SO₄ yielded 100 mg. 7,8-dihydroxanthopterin (III), analyzed as III.O.5H₂SO₄.0.5H₂O, λ_{maximum} 276, 305 m μ , E_{max}. 11700, 8700,

λ_{\min} . 297 $m\mu$ (at pH 1), λ_{\max} 276, 310 (inflection) $m\mu$, E_{\max} . 11300, 5300 (at pH 11). 2,4-Diamino-7-hydroxy-6-pteridinecarboxylic acid (IV) (5 g.) in 100 cc. 2 N aqueous NaOH was shaken 20 min. at room temperature with 10 g. Zn dust, then heated to 50°, filtered, and the warm filtrate acidified with 12 cc. concentrated HCl and cooled to yield 3.8 g. 5,6-dihydro derivative (V) (with 1 mol. H₂O) of IV, λ_{\max} 298, 336 $m\mu$, E_{\max} . 11200, 12700, λ_{\min} . 265, 310 $m\mu$ (at pH 1); λ_{\max} 255, 342 $m\mu$, E_{\max} . 11800, 13400, λ_{\min} . 250, 295 $m\mu$ (at pH 11), also obtained by reduction of IV in aqueous NaOH with Na-Hg, together with 250 mg. of a compound C₇H₁₀N₆O₄, λ_{\max} 280, 335 $m\mu$, E_{\max} . 12100, 2500 (at pH 1), λ_{\max} 278, 340 $m\mu$, E_{\max} . 8000, 2900 (at pH 11), presumably formed by hydrolytic ring opening of V. V heated 2 hrs. at 140° lost H, CO₂, and H₂O to give a crude product C₆-H₈N₆O (VI). To 90 mg. VI in 1 cc. 2 N NaOH was added slowly 8.4 cc. 0.04 M aqueous KMnO₄, the excess removed with Na₂SO₃, the mixture filtered, and the filtrate acidified with AcOH to pH 5 to give 55 mg. 2,4-diamino-7-hydroxypteridine, λ_{\max} 295, 338 $m\mu$, E_{\max} . 12200, 14400; λ_{\min} . 265, 310 $m\mu$ (at pH 1), λ_{\max} 257, 340 $m\mu$, E_{\max} . 12000, 14100, λ_{\min} . 250, 290 $m\mu$ (at pH 11). Reduction of isoxanthopterine-6-carboxylic acid (VII) in 2 N NaOH with Zn dust gave a mixture of 5,6-dihydro derivative of VII, 5,6-dihydroisoxanthopterine, and isoxanthopterine (VIII); the reduction of VII carried out at 150° gave VIII, λ_{\max} 288, 340 $m\mu$, E_{\max} . 10000, 13100, λ_{\min} . 260, 302 $m\mu$ (at pH 1), λ_{\max} 250, 275 (inflection), 342 $m\mu$, E_{\max} . 10000, 3600, 12700, λ_{\min} . 245, 290 $m\mu$ (at pH 11). 2-Amino-5-chloroacetamido-4,6-pyrimidinediol-H₂O (300 mg.) and 230 mg. NaHCO₃ in 10 cc. H₂O heated 1 hr. in a water bath and the mixture acidified with AcOH to pH 5 and cooled yielded 145 mg. 2-amino-4,6-dihydroxy-p-oxazino[2,3-d]pyrimidine-4,6-diol-H₂O, λ_{\max} 258, 308 $m\mu$, E_{\max} . 12400, 9800, λ_{\min} . 280 $m\mu$ (at pH 1), λ_{\max} 267, 300 (inflection) $m\mu$, E_{\max} . 11800, 8000 (at pH 11). I (1 g.) was heated 20 hrs. at 120° with 25 cc. concentrated NH₄OH in a sealed tube, the excess NH₃ evaporated on a steam bath, the residue (320 mg.), which showed the same absorption spectrum as I, filtered off, and the filtrate acidified with AcOH to give a precipitate with the same spectrum

as

the degradation product from I and Ba(OH)₂. Condensation of 2,4,5-triamino-6-pyrimidol (IX)-2HCl with (CHO)₂ at 70° yielded a diglyoxalyl derivative (X) of IX, λ_{\max} 235, 270, 330 $m\mu$ at pH 1. X dissolved in 2 N NaOH and precipitated with acid gave 2-amino-4-pteridinol

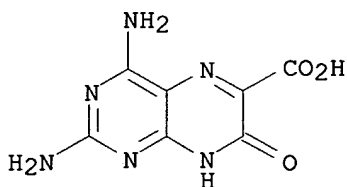
(XI),

λ_{\max} 312 $m\mu$, E_{\max} . 8150, λ_{\min} . 270 $m\mu$ (at pH 1), λ_{\max} 252, 358 $m\mu$, E_{\max} . 22000, 7600, λ_{\min} . 295 $m\mu$ (at pH 11). X gave with 2 mols. PhNHNH₂ a phenylhydrazone, C₂₀H₁₉N₉O. To 100 mg. 2,4,5-triamino-6-carboxymethoxypyrimidine suspended in 10 cc. H₂O was added 0.3 cc. 30% aqueous (CH₂O)₂ and 0.6 cc. 2 N NaOH, the mixture let stand 2 hrs. at room temperature, then heated 45 min. on a steam-bath (the resulting solution gave at pH 1 a spectrum almost identical with that of X, at pH 11 with that of XI), let stand overnight at room temperature, evaporated in a stream of

air to 6 cc. and chilled to yield 58 mg. 2-amino-4-(carboxymethoxy)pteridine, λ_{\max} 313 $m\mu$, E_{\max} . 7700, λ_{\min} . 270 $m\mu$ (at pH 1), λ_{\max} 252, 360 $m\mu$, E_{\max} . 21200, 7100, λ_{\min} . 290 $m\mu$ (at pH 11). 6-Chloro-2,4-diaminopyrimidine, λ_{\max} 298 $m\mu$ (at pH 1), λ_{\max} 282 $m\mu$ (at pH 11) (2.35 g.), and 2.15 g. NaOCH₂COEt in 8 cc. HOCH₂CO₂Et heated 14 hrs. at 110°, the mixture cooled, diluted with 100 cc. dry Et₂O, filtered, the residue leached with 50 cc. absolute EtOH, and the extract evaporated to dryness dissolved in 17 cc. H₂O gave a solution of 6-carbethoxymethoxy-2,4-diaminopyrimidine (XII), λ_{\max} 276 $m\mu$, O.D. 0.99 (at pH 1), λ_{\max} 275 $m\mu$, O.D. 0.75 (at pH 11). To the

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aqueous solution of XII was added p-ClC6H4N2Cl (from 220 mg. p-ClC6H4NH2 and
125 mg. NaNO2) and 2 g. NaHCO3, and the mixture let stand at 0° overnight
to give 6-carbethoxymethoxy-5-(p-chlorophenylazo)-2,4-diaminopyrimidine
(XIII), bright yellow solid. XIII (100 mg.) in 20 cc. 50% aqueous EtOH boiled
5 min. with 500 mg. Zn dust and 2 cc. 2 N HCl, filtered, the filtrate made
alkaline with 3 cc. 2 N NaOH, filtered, and the filtrate acidified with AcOH
to pH 5 yielded 23 mg. I, λ_{maximum} 263, 312 m μ , Emax. 13200, 8800,
 λ_{min} . 290 m μ (at pH 1); λ_{maximum} 275 m μ , Emax. 13700 (at
pH 11).
IT 2521-97-3P, 6-Pteridinecarboxylic acid, 2,4-diamino-7-hydroxy-
RL: PREP (Preparation)
(preparation of)
RN 2521-97-3 CAPLUS
CN 6-Pteridinecarboxylic acid, 2,4-diamino-1,7-dihydro-7-oxo- (9CI) (CA
INDEX NAME)



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L6 0 S L4 AND PENTANE?

L7 16 S L4 AND (CARBOXYL? OR PETANEDIOIC)

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COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY

TOTAL
SESSION

CA SUBSCRIBER PRICE

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